"Quantum For All"
Q-Lab Town Hall

March 3, 2022

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Agenda

- Q-Lab Seed Grant Overview
- Quantum vs. Classical Computing
- Applications & Exemplars
- Resources
- Q&A

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National Quantum Laboratory (Q-Lab)

- **Launched in September 2021 in partnership with IonQ**
  - *UMD is a world leader in quantum technologies and computing*
  - *IonQ is a leading developer of quantum computers*
- *Focus on developing near-term applications for Noisy, Intermediate-Scale Quantum (NISQ) computers*
  - Finding "killer apps" for QC requires co-development with end-users
- *Q-Lab Partnership Includes:*
  - Enabling broader access to technical expertise and practical QC resources across the UMD ecosystem
  - Access to more powerful QC systems in development than available via cloud providers
  - Co-location of researchers and IonQ to enable collaborative development of applications, to include potential optimization of prototype systems

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Q-Lab Seed Grant

- **$300k total**, plus access to Q-Lab time
- *Three Types of Award:*
  - ***Exploratory Research*** *– Engaging non-quantum scientists with QC ($20k)*
  - ***Proof of Concept*** *– QIS experts working on NISQ-era applications ($40k)*
  - ***Curriculum Development*** *– Supports range of training & education ($10k)*
- **Proposals Due**: March 27, 11:59 pm EST
- **Eligibility**: Faculty (TTK & PTK), limited to 1 research & 1 curriculum
- **Quantum Expertise**: Not required for PI. Partnering with a quantum expert is *very strongly encouraged*, but note that seed grant funds must stay inside the university

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Q-Lab Seed Grant Process

- **Review RFP and apply on UMD's InfoReady portal**

- **Required Application Materials**
  - Completed Universal Funding Form (50% cost-share)
  - Project Narrative (up to 3 pages + references)
  - Q-Lab Resources Request, if any
  - Budget & Justification
  - Biosketches (up to 2 pages each)

Write for a general audience that might not be familiar with your field of study

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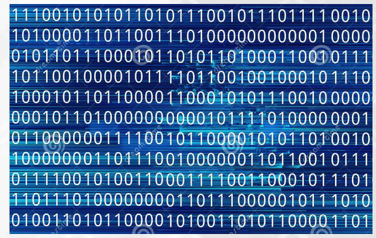
Inspiration | Boldness | Curiosity | Passion

Classical computing or quantum computing?



Modern-day digital computers

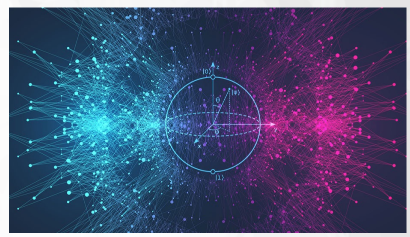
- ✓ extremely powerful
- ✓ backbone of the Information Age
- ✓ very high precision for arithmetic and algebraic calculations – anything yielding certain outcome

… all based on manipulating long strings of '0' and '1' (bits)

- limited when it comes to probabilistic problems:
  - probability distributions not or barely known or are complicated functions
  - data fitting may yield local minima instead of the global minimum
  - large number of parameters often result in exponential growth of complexity
- Random numbers (obtained via mathematical algorithms) are not completely random
  → large samples of random numbers won't cover the probability space equally
  → cybersecurity keys and encrypted data can – in principle – be decrypted by a third party

Quantum systems

- ➢ inherently probabilistic
- ➢ populate all possible states simultaneously
- ➢ quantum objects superpose (interfere) and can act coherently (entangled)
- ➢ number of possible states increases exponentially (2^N for N qubits)



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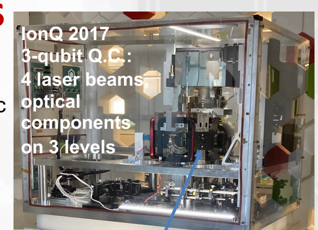
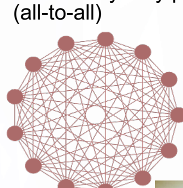
Today's quantum computers

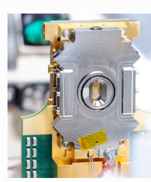


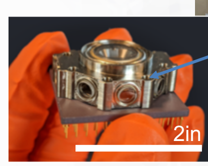
many different implementations!

Ion-trap Q.C. (ions placed in quadrupole & oscillating electric field, requires high-vacuum chambers)

- induced excitation of individual atoms (Ytterbium, Barium)
- manipulation by lasers (one for each qubit & one global)
- connectivity: any pair (all-to-all)

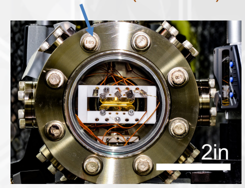


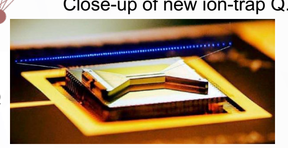




Close-up of new ion-trap Q.C. & vacuum chamber

Vacuum chamber (10^{-11} Torr)



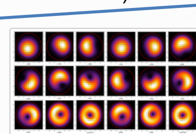


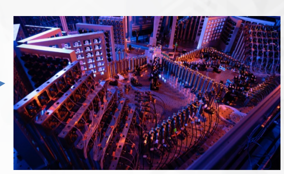
new IonQ 32-qubit Q.C.

Ion-trap Q.C. also: Honeywell, UMD/JQI, U.Innsbruck, …

other implementations, e.g.:

- neutral atom traps (trapped in potential wells)
- photonic networks
- quantum dots (nanoparticles in ^{28}Si at T~1.0K, spins manipulated by microwaves)





USTC, Shanghai: 144-modes photon interferometer

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Today's quantum computers (cont.)

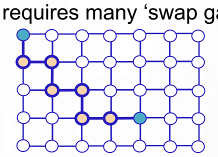
Superconducting QC

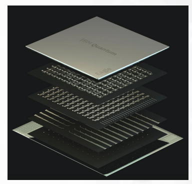
- Cooper pairs (electron pairs in anharmonic oscillator, operated at T ~15mK)
- Limitations:
- energy fluctuations at T > 160mK (Cooper pairs unstable)
- coherence times ~100 μsec

→ place 3 (or 9) qubits together for error correction
(only works for uncorrelated Copper pair breaking)

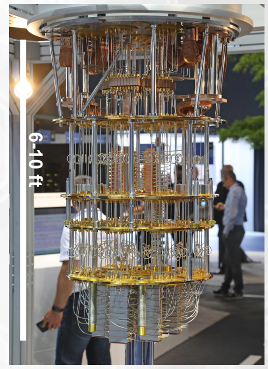
- connectivity only to nearest neighbors

→ requires many 'swap gates'





IBM Eagle 127 qubits

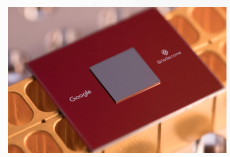


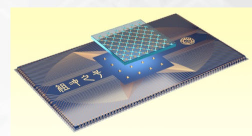
IBM, similar: Intel, AMD, Google, Microsoft, PsiQuantum, …

- today's NISQ computers
(noisy intermediate-scale quantum era)
- consider the first logic gates and digital computers in 1940s/50s

- **better by 2024/5 ?**

- ion/atom traps: 256 to 512 qubits
- quantum dots: 64 to 144 qubits
- superconductors: 512 to 1024 qubits





Google Bristlecone 72 qubits, Juizhang 113 qubits

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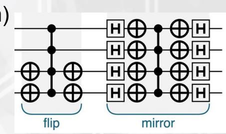
Basic quantum algorithms

- **Method**:
- access hidden patterns stored in phases and amplitudes of quantum registers via phase manipulations and computing in superposition
- **Challenges**:
- how to get a signal into a quantum register? (initializing input registers)
- how to access the results ("uncomputing" required to disentangle qubit registers)

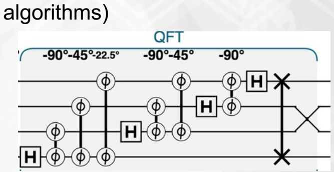
1) Amplitude Amplification (QAA: generalization of Grover's algorithm)

- convert phase differences within a quantum register into detectable variations in magnitudes via repeated phase flip & mirror operations
- probabilities fluctuate in QAA iterations → optimal number of iterations $N_{AA} \approx \frac{\pi}{4}\sqrt{\frac{2^n}{m}}$ (where *n*=number of qubits, *m*=number of marked (flipped) values)



2) Fourier Transform (QFT: core of many powerful quantum algorithms)

- allows to read out the frequency with which values vary; mirror-image peaks whenever the phase shifts by 180°
(precision relative to 2*n* (where *n*=number of qubits))
- more complex signals produce superposition of frequency values → rerun QFT multiple times



3) Phase Estimation: (QPE): returns the superposition of all eigen-phases of an operation *U*, applies inverse QFT; best results if eigenstates given as input.

- output register contains ${}^{\vartheta_j}/_{360} \times 2^m$ (where *m*=size of output register) → estimate the eigen-phase ϑ_j to *p* bits precision and probability of error ε : size of output reg. $m = p + \lceil \log(2 + \frac{1}{\varepsilon}) \rceil$

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Potential applications

McKinsey Report 12/21

Four types of use cases:

1) Quantum simulation of quantum-mechanical systems or processes (Q.C. inherently suited for such intractable quantum simulations).

2) Quantum linear algebra, mostly applied in AI and ML, esp. NLP, but also PDE;

mainly hybrid computation: speed-up time-expensive components of conventional methods.

3) Quantum optimization: solve complex problems, esp. discrete optimization, e.g. generative design, traffic management, portfolio optimization, unstructured database searches, improved Monte Carlo simulations

4) Quantum factorization: cybersecurity

Lighthouse use cases along the quantum-computing hardware development timeline

Development timeline: Not fully error corrected ← → Fully error corrected

Current state of development

	Early stage	Late stage	Fault-tolerant early stage	Fault-tolerant late stages	Universal quantum supercomputer[2]
Proxy for hardware needs,[1] qubits ● Annealing ● Gate-based QC	Logical: N/A ● ~10,000 ● ~100	Logical: N/A ● ~100,000 ● ~1,000	Logical: ~100 ● ~100,000 ● ~100,000	Logical: ~1,000 ● ~1,000,000 ● ~1,000,000	Logical: ~10,000+ ● ~10,000,000+ ● ~10,000,000+
Challenges for gate-based quantum computing		Scalability and error correction			Quantum data storage (quantum RAM) and efficient data input and readout
Challenges for annealing		Better qubit connectivity			
Lighthouse use cases Algorithm archetypes: Linear algebra (AI/ML); Optimization; Simulation; Factoring; Other Industries: Pharmaceuticals; Chemicals; Automotive; Finance; Logistics	Certified randomness (Job) scheduling optimization Route and fleet optimization Clinical-trial site-selection optimization	Synthetic-data generation Approximate QM simulation[3] Small-scale quantum reinforcement learning Collateral and portfolio optimization Robot path optimization Production-process optimization	Light risk simulation (Approximate) MD,[3] MM[3] simulation (eg, protein folding) Trading-strategy optimization Protein folding	Breaking RSA cryptography Financial and cyberrisk simulation Large-molecule simulation ADME[4] and toxicity prediction Complex-mixture simulation Solid-material simulation Catalysis or synthesis optimization Finite element method Supply-chain optimization	Supply-chain-disruption modeling Self-driving robots Credit-risk management Financial-crime detection Personalized medicine Automated drug recommendations Multiscale production optimization

[1]Physical qubits needed to achieve 1 logical qubit per technology, based on current error rates for superconducting qubits.
[2]Use cases will combine algorithm archetypes or the archetype is not yet confirmed.
[3]QM: quantum mechanics; MD: molecular dynamics; MM: molecular mechanics.
[4]Absorption, distribution, metabolism, and excretion.

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Algorithms and techniques:

a) Quantum Simulation:

- class of procedures that efficiently implement QPU operations for representing Hermitian matrices by breaking down a matrix into a sequence of 'easier-to-encode' matrices: $H = H_1 + H_2 + \cdots + H_n$
- **Variational Quantum Eigensolver** (VQE: application of Ritz' variational theorem)
- applications: quantum physics, quantum chemistry e.g. optimizing catalytic processes: nitrogen fixation, carbon sequestration, protein folding

b) Quantum Annealing:

- find global minimum for combinatorial problems with many shallow local minima
- applications: traveling salesman problem, complex materials/solids, classification problems

c) Quantum Search:

- modified QAA to evaluate boolean sequences (yes/no questions).
- **Quantum Approximate Optimization Algorithm** (QAOA: yield expectation value from sampling constraint by a cost function)
- applications: search in unstructured databases, combinatorial optimization, oracle functions, boolean satisfiability

d) Quantum Linear Algebra: HHL algorithm (Hallow,Hassidim,Lloyd 2009)

- solve systems of linear equations via eigendecomposition of the coefficients matrix → amplitude-encoded solution (individual solutions are hidden in amplitudes of the superposition, but derived properties of solution can be extracted: mean, sum, frequency components in solutions, etc)
- applications: computational methods

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Algorithms and techniques (cont.):

e) Quantum machine learning (need ~30+ qubits)

- **dimensionality reduction: qPCA** → find eigendecomposition of the covariance matrix (represented as density operator)
- **supervised ML: qSVM** → amplitude encoding of hyperplane parameters and least-square optimization
- **others** (need ~50+ qubits): linear regression, re-enforcement learning, Boltzmann machines, quantum auto-encoder, quantum recommender system, …
- applications: multi-robot path planning, real-time traffic management, autonomous vehicles, finance portfolio & risk management, fraud-prediction modeling, cyber-risk management, …

f) Quantum Image Processing

- analyzing phases in superposition (QAA iterations with inverse QFT)
- applications: supersampling, ray-tracing engines, pixel shader, figure alignment/registration

g) Shor's factoring algorithm

- determines periodicity of a periodic function for possibly complicated periodicity (hidden subgroup problem) using QFT as coprocessor
- applications: period finding, order finding, discrete logarithms → RSAinteger factorization

Resources:

- tutorials and help to get started with quantum computing: https://community.qiskit.org/textbook ; https://projectq.readthedocs.io/en/latest ; https://www.machinelevel.com/qc/doc/qcengine_workbench.html ; https://ionq.com/get-started ; https://quantum-computing.ibm.com and many more …
- UMD quantum initiatives (next slide)

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Quantum Initiatives at UMD

- **Joint Quantum Institute** (jqi.umd.edu), founded in 2006 in partnership with NIST and LPS, is an internationally renowned center for groundbreaking research in quantum science, from theory to experiment.
- **Joint Center for Quantum Information and Computer Science** (https://quics.umd.edu) is a collaboration with NIST that expands research at the junction of quantum physics, computer science and information theory.
- **Quantum Technology Center** (qtc.umd.edu) joins researchers in engineering and physics to focus on translating quantum physics into innovative technologies.
- **Quantum Materials Center** (qmc.umd.edu) explores existing superconductors, as well as the study and creation of quantum materials to enable new devices.
- **Institute for Robust Quantum Simulation** (rqs.umd.edu) explores the theoretical foundations of quantum algorithms and error correction as well as experimental implementations of quantum simulations.
- **LPS Qubit Collaboratory** (www.qubitcollaboratory.org), hosted at NSA's Laboratory for Physical Sciences (LPS) at UMD, pursues collaborative research and innovative workforce development programs.
- **Quantum Startup Foundry** (quantum.umd.edu/startup) brings together the resources to support entrepreneurs and startups in accelerating the time to bring quantum technologies to market.
- **Mid-Atlantic Quantum Alliance** (mqa.umd.edu) serves as an inclusive forum to engage and collaborate on research, education, global thought leadership, and building a vibrant and diverse ecosystem to support quantum innovation.
- **National Quantum Lab** (glue.umd.edu/hpcc/qlab), a new user facility in partnership with IonQ, provides unique research and teaching opportunities using innovative technologies in the field of quantum computing.
- **Mid-Atlantic Regional Quantum-Internet** (**MARQI**), a new quantum network enabling quantum computers to communicate over large distances on the internet while preserving quantum coherence (entanglement).

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Q-Lab (National Quantum Lab)

User facility of UMD in partnership with IonQ, being established (4505 Campus Drive)

Coming soon! (April/May 2022)

Mission:

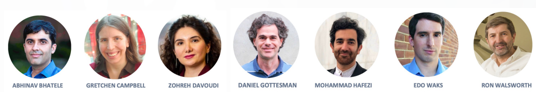
- offer training (bootcamps, workshops, classes) in quantum computing
- provide privileged access to IonQ's trapped-ion quantum computers
- advance research in early applications of quantum computers and quantum networks
- connect researchers from multiple disciplines with interest in these fields
- mentor tomorrow's experts in quantum computing, its application and technical realization

Questions?
Contact:
fklein@umd.edu

- Quantum track on this year's UMD hackathon!
- Seed Grant program for graduate research

IonQ API tokens limited to active members of the UMCP community; users are not allowed to share IonQ API tokens with anyone outside the UMCP community!

Advisory Committee:



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QC App Finance

"**Multiverse Computing** today announced a partnership with **IonQ**, the leader in trapped-ion quantum computing, which will **enable financial services organizations to model risk more accurately and quickly** than ever before using the IonQ Quantum Cloud platform within Singularity®, Multiverse's financial solution." – *Nov 21, 2021*

"Rigetti began providing much wider access to its 80-qubit system (Aspen-M), announced a **collaboration with Nasdaq** to develop FS apps. […] The collaboration will focus on 'machine learning, optimization and simulation problems with Nasdaq's market perspective, domain expertise and data,' […] The collaboration will **evaluate financial applications that 'may benefit from the ability of quantum computing** to solve computational problems with improved accuracy, speed, or cost.'" – *Feb 17, 2022*

1

QC App Logistics

"**Quantum-South**'s team has been working in **container load optimization for air cargo since** the **Airbus** Quantum Computing Challenge in 2019 where it became one of the global finalists. Airbus has identified this problem as one of the most challenging in the aerospace industry." – *Feb 14, 2022*

2

QC App Pharma

"**Cambridge Quantum** is pleased to announce their collaboration with **Roche** to design and implement noisy-intermediate-scale-quantum **(NISQ) algorithms for early-stage drug discovery and development**." – *Jan 29, 2021*

SEEQC, the Digital Quantum Computing company, today announced its UK-based team has been awarded a £6.85M grant from Innovate UK to **build a commercially scalable application-specific quantum computer** designed to **tackle prohibitively high costs within pharmaceutical drug development**. – *Nov 5, 2021*

3

BMW QC Challenge

1. Sensor positions for automated driving functions: Accenture's winning team tackled the problem of optimising the positioning of sensors for highly automated driving functions.

2. Simulation of material deformations: The jury concluded that the quantum computing start-up Qu&Co stood out with its approach to solving partial differential equations in the field of numerical simulation.

3. Configuration optimisation of pre-series vehicles: The winning team from 1QBit and NTT came out on top with hybrid algorithms for solving satisfiability problems in propositional logic for optimising equipment configuration.

4. Automated quality analyses: The QC Ware team stood out with its approach, drawn from the field of machine learning, that can be used in image recognition in the area of quality analysis.

4

QSF TraQtion

QuantFi
Quantum Computing For Finance

- Collaborations in the areas of distribution loading, QAOA, QML, Quantum Monte Carlo
- Working with professors/their PhD students on algorithm development for financial and actuarial use cases.

CLASSIQ

- Collaborations to automatically synthesize high-level models into optimized quantum circuits

QUANTUM FLYTRAP

- Collaborations to make quantum computing applicatins more accessible through better user interface design

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